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Title: Energy Transport in Nonlinear Systems: From Flux Networks to Energy Landscapes

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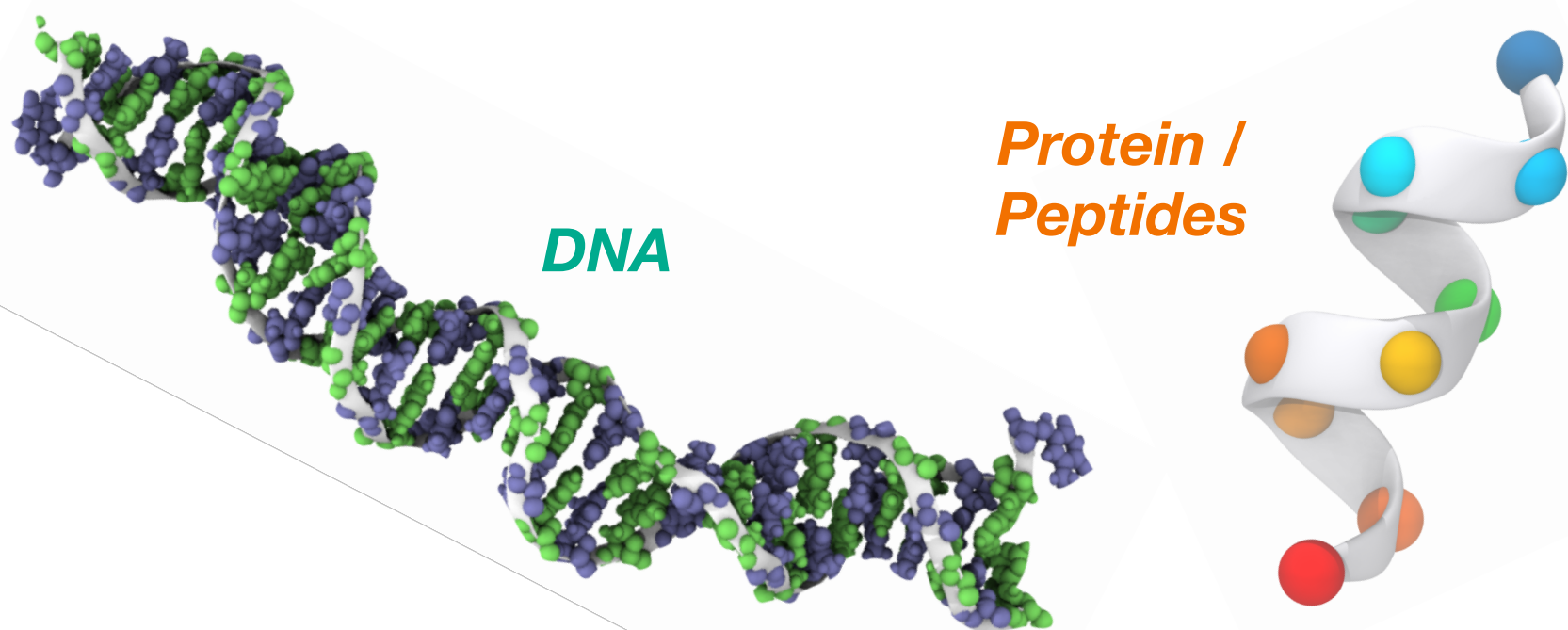
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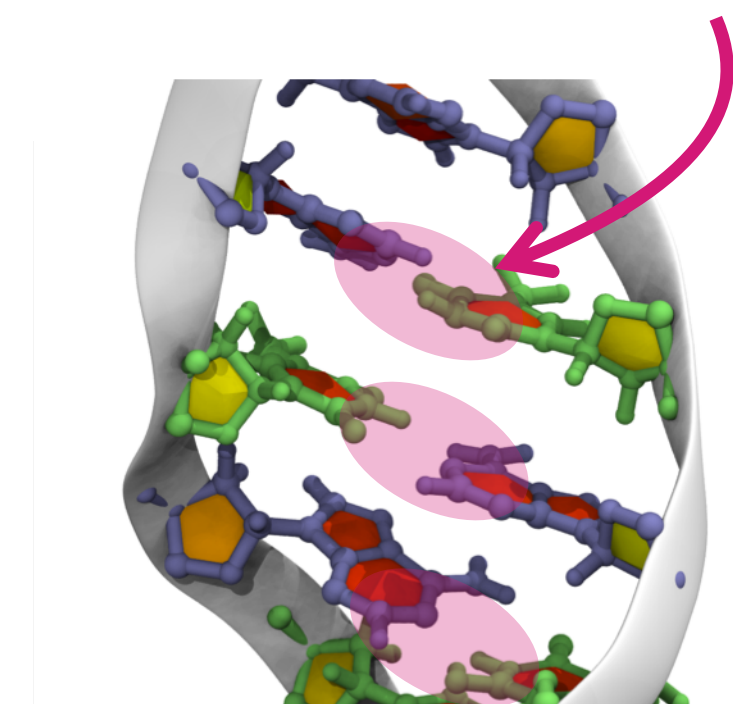
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# 1. Thermal transport reflects protein dynamics and DNA denaturation by probing nonequilibrium aspects of free energy landscapes.



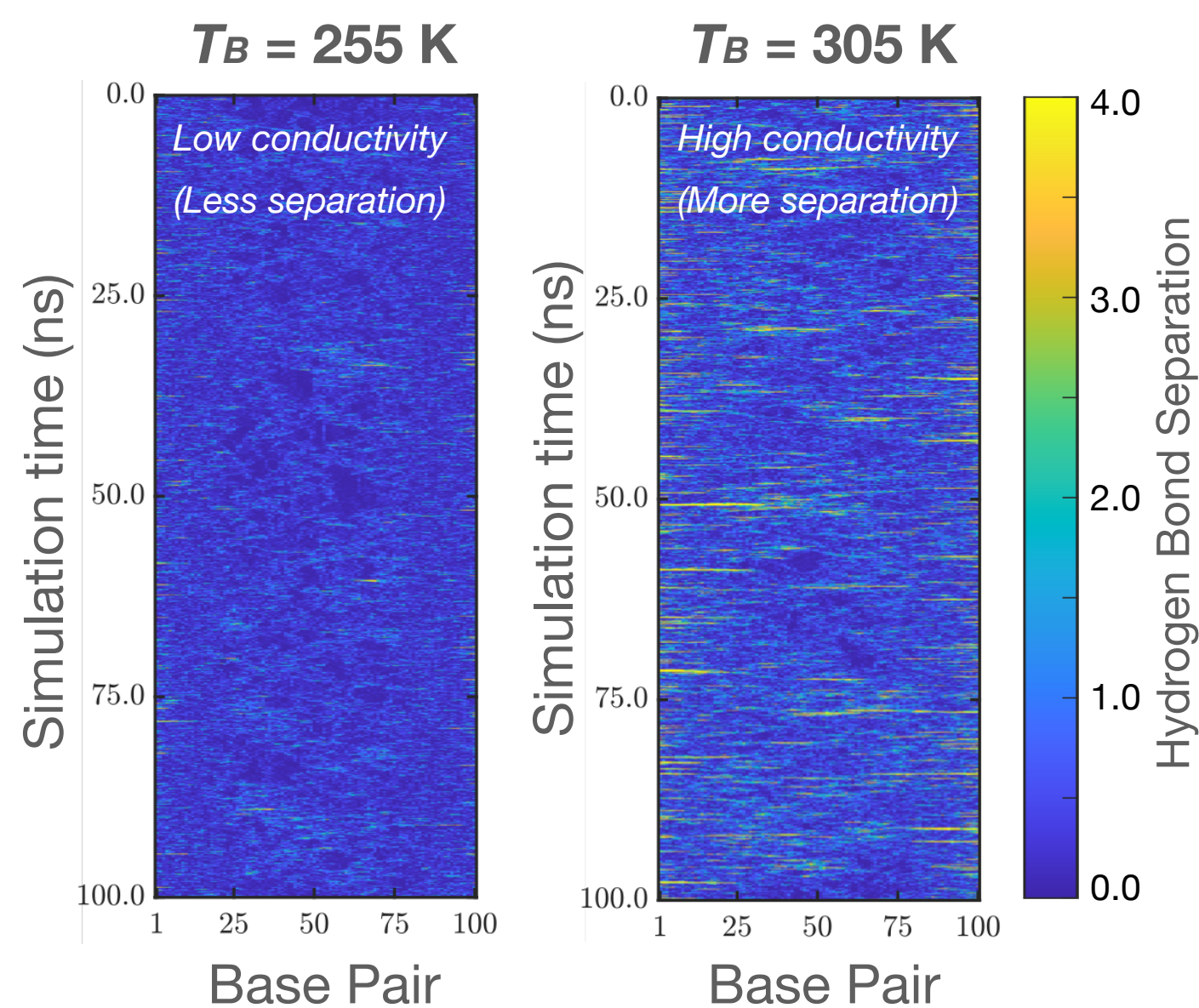
These provide robust and general models for nonlinear phenomena in complex materials.

# 2. DNA melting is quantified through the hydrogen bond distance between paired nucleic acid strands in DNA.



Strand separation increases with temperature ( $T_B$ ) — we describe this using molecular dynamics and effective, coarse-grained (CG) models (bead-spring / PBD).

*In this context, transport probes nonlinearity & reflects energy landscape architecture.\**

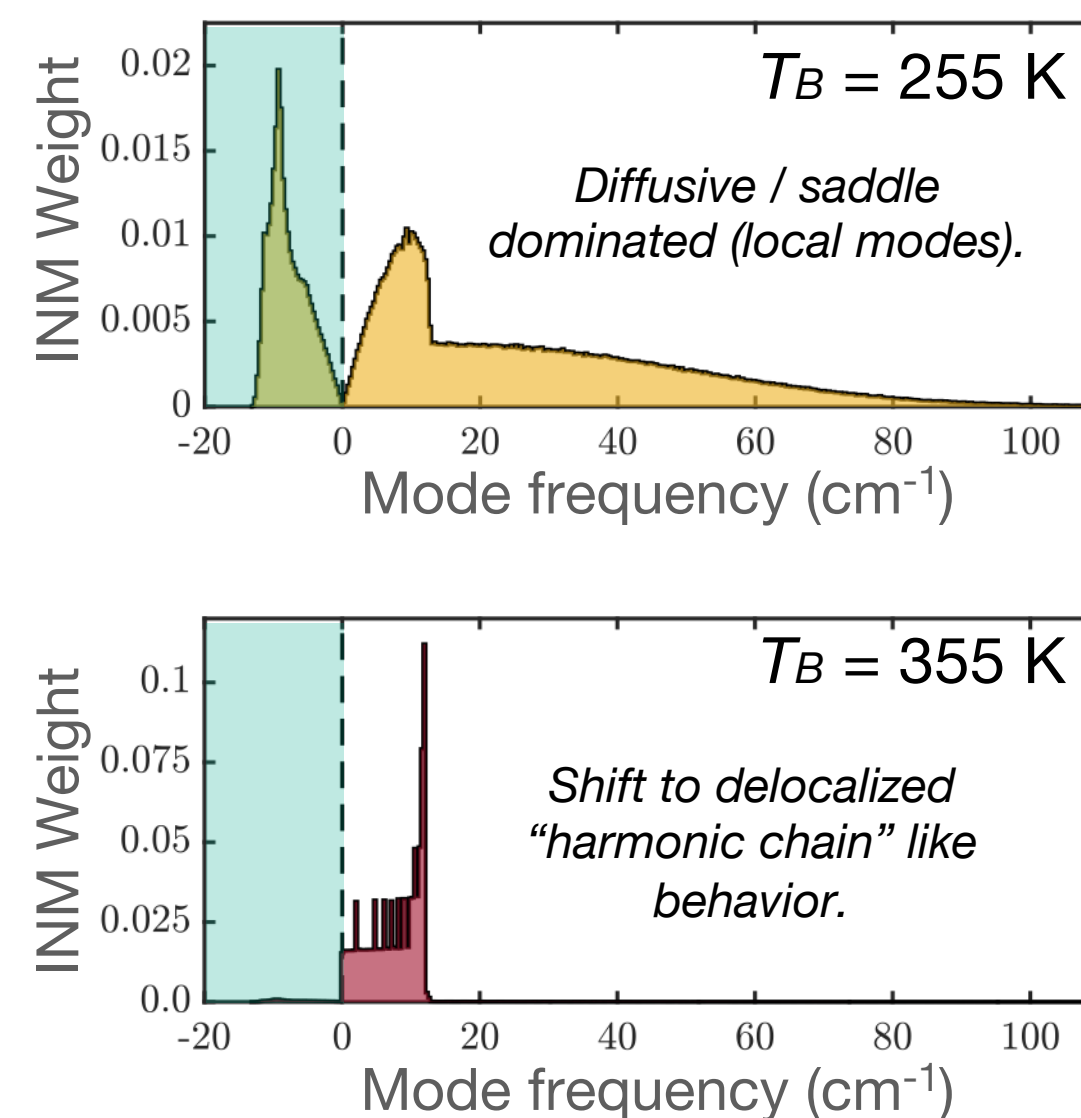


Microsecond-scale simulations of heat conduction in a DNA model with thermal gradient of  $\Delta T = 10\text{ K}$  across the strand. The strands separate (or “melt”) at higher bath temperatures ( $T_B \gg 355\text{ K}$ )

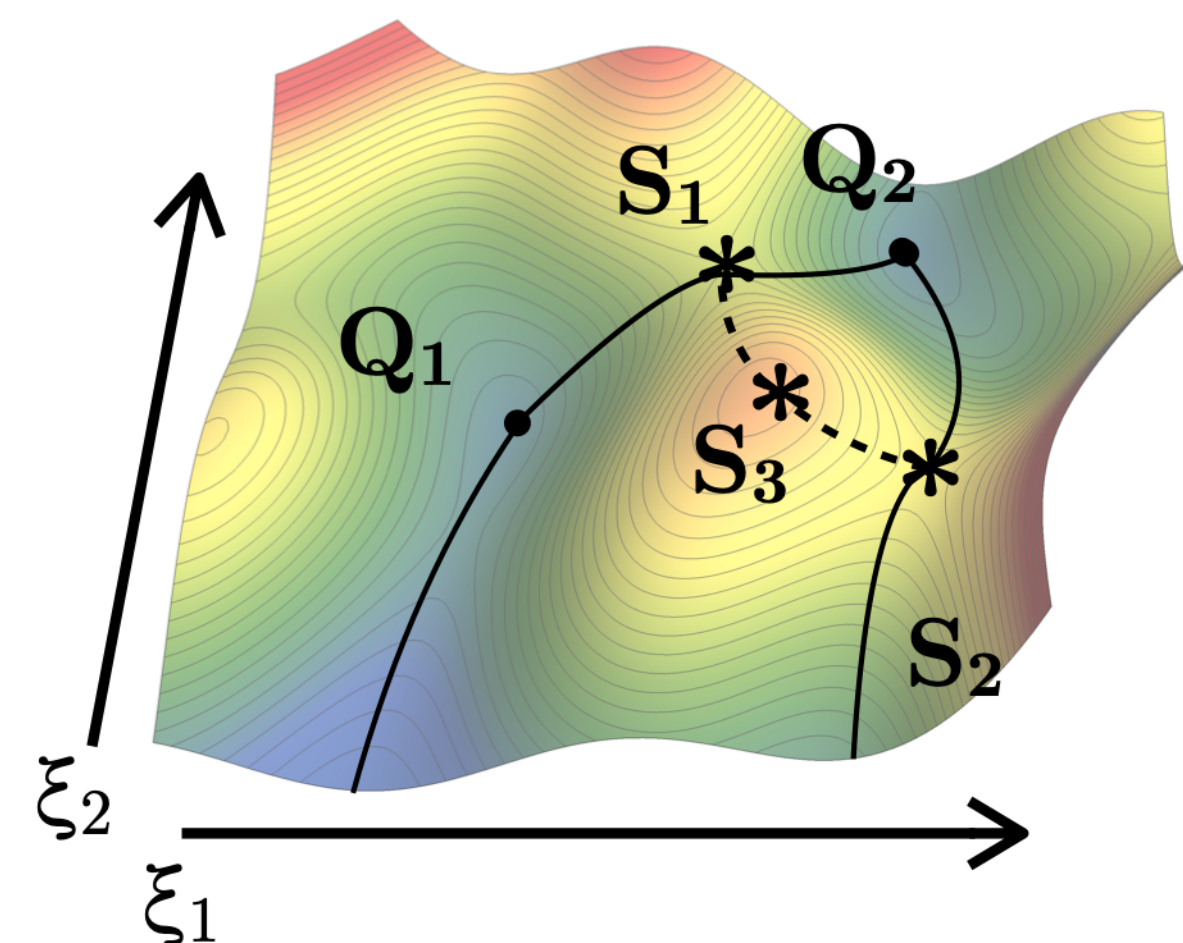
# Energy Transport in Nonlinear Systems: From Flux Networks to Energy Landscapes

PI: Kirill Velizhanin (T1)

# 3. Instantaneous Normal Modes reflect energy landscape architecture during steady-state heat transport.



Modes with **imaginary frequency** associated with saddles / barrier crossing or ‘shoulders’ in the free energy landscape.



High temperature transport is via delocalized, phonon-like modes:

*Energy scale is above landscape features associated with nonlinearity.*

\*J. E. Elenewski, K. Velizhanin, M. Zwolak, *Nat. Commun.* **10**, 4662 (2019)